201-16554Q

IUCLID

Data Set

Existing Chemical	:	ID: 111381-90-9
Memo	:	HPV Chemical
CAS No.	:	111381-90-9
TSCA Name	:	1,2-Benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Synonym	:	1,2-benzenedicarboxylic acid (C7,C11) ester, branched and linear

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	05.07.2006
Revision date	:	
Date of last update	:	05.07.2006
Number of pages	:	32
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers: 68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6 and 111381-90-9 (see remark for names)

Remark : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers and names:

68515-50-4 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear (DHP)

71888-89-6 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (DIHP)

27554-26-3 1,2,-benzenedicarboxylic acid, diisooctyl ester (DIOP)

68515-44-6 1,2-benzenedicarboxylic acid, diheptyl ester, branched and linear (DinHP)

111381-89-6 1,2-benzenedicarboxylic acid (C7, C9) ester, branched and linear (79P)

111381-90-9 1,2-benzenedicarboxylic acid, (C7,C11) ester, branched and linear (711P)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower molecular weight transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate subcategories. Of the phthalates in this subcategory, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

03.04.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	< -50 °C
Decomposition	:	no, at °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Remark	:	Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited informtion on how the data were developed.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (11)

Value	:	85 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(3) invalid

18.04.2006 (5)

2.2 BOILING POINT

Value	:	440 °C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
18.04.2006 (5)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .000000068 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including a dinonyl phthalate, which provided an intermediate value for a heptyl undecyl phthalate ester.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for dinonyl phthalate ester was 564.8 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
18.04.2006 (3)

Value	:	.0000003 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

18.04.2006 (5)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	8.6 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dinonyl phthalate, which provided an intermediate value for a heptyl undecyl phthalate ester. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for dinonyl phthalate ester was 564.8 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths

from 1 to 13 carbons.

Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

18.04.2006 (3)

Partition coefficient	:	octanol-water
Log pow	:	9.37 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

18.04.2006 (5)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	.00031 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dinonyl phthalate, which provided an intermediate value for a heptyl undecyl phthalate ester.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for dinonyl phthalate ester was 564.8 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
18.04.2006 (3)

Solubility in : Water
Value : .00002 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 9.37.

Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

05.07.2006 (5)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.0000000000248 cm³/(molecule*sec)
Degradation	:	50 % after 5.2 hour(s)
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	:	50% degradation after 5.18 hrs or 0.432 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

12.05.2006 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	4.2 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint
12.05.2006		(5)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level I
Year	:	
Remark	:	Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	418.62
Temperature	25° C
Log Kow	8.6
Water Solubility	0.00031 g/m3
Vapor Pressure	0.0000068 Pa
Melting Point	-50°C (used in calculation; reported value is <-50°C)

Result	:	Using the Mackay Level I calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance	:	CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint
18.04.2006		(7)
Media	:	air - biota - sediment(s) - soil - water
Method	:	Calculation according Mackay, Level III
Year	:	

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	418.62
Temperature	25° C
Log Kow	8.6
Water Solubility	0.00031 g/m3
Vapor Pressure	0.0000068 Pa
Melting Point	-50°C (used in calculation; reported value is <-50°C)

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	10.4a
Water	240b
Soil	840c
Sediment	840c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on read-across biodegradation data from two phthalate esters: 1,2-benzenedicarboxylic acid, di-C7 alkyl esters (CAS No. 71888-89-6); Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report. 1,2-Benzenedicarboxylic acid, diundecyl ester (CAS No. 3648-20-2); Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear:

Compartment	% Distribution
Air	0.4
Water	5.3
Soil	65.8
Sediment	28.5

Test substance : CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester,

branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
12.05.2006 (7)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: Adapted domestic sewage and soil
Concentration	:	20 mg/l related to Test substance related to
Contact time	:	28 day(s)
Degradation	:	= 98 (±) % after
Result	:	
Deg. product	:	
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Method/Guideline - USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum - Domestic sewage and soil. Kinetics - Not Reported Degradation Products - Not Reported Analytical Monitoring - Yes
Result	:	Concentration - Nominal test concentration = 20 mg/L for test substance and glucose. Units - % biodegradation Result - >99% primary biodegradation and 98% (s.d. +/-2%) ultimate biodegradation. Primary degradation is expressed as the loss of test substance based on analytical measurements of parent test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 (based on test substance) evolved in each flask.
Test condition	:	Test Conditions - Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120 rpm at 22 +/- 2 deg C.
Test substance	:	1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear . (CAS# 111381-90-9) Synonym: 711P No information on purity, but 711P was analytically confirmed to be within commercial specifications.
Conclusion	:	The substance can biodegrad to a high extent using an acclimated

population of microorganisms obtained from a sewage treatment system and soil.

Reliability : (1) valid without restriction
This summary is rated a "1" because it followed a USEPA standard guideline, which describes a procedure specifically designed to evaluate biodegradation under acclimated conditions, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
27.04.2006 (13)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> .21 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1975
GLP	:	yes
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial concentration.
Result	:	96 hr LC50 >0.21 mg/L Mean measured values were used in the LC50 calculation. Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29 mg/L. Mean measured test concentrations: <0.0083, 0.019, 0.041, 0.049, 0.092, and 0.21 mg/L. Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period. No mortality occurred in any treatment level during the 96-hour exposure. A film of undissolved test substance was observed in the highest treatment level at 24 hours only. Droplets of undissolved test substance were observed in the three lowest treatment levels at 24 hours only. The highest nominal loading was in excess of the water solubility of this test substance, which indicates that the test substance is not acutely toxic at its saturation limit. % Mortality results at 96 hrs per replicate for control and treatment levels: Conc. (mg/L) Rep1/Rep2 Control 0 / 0 0.019 0 / 0 0.041 0 / 0 0.049 0 / 0 0.092 0 / 0 0.21 0 / 0
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15 L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.

Fish mean length = 62 mm and mean wet weight = 2.3 g. Test temperature = 11 Deg C. The pH ranged from 6.9 to 7.5. The mean dissolved oxygen ranged from 8.9 to 9.1 mg/L. Ranges of total hardness and alkalinity as CaCO3 of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively.

Fish were obtained from a Montana supplier.

Test substance : 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear (CAS# 111381-90-9)
Purity: 100% active ingredient

Conclusion : Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

27.04.2006 (4) (12)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : > .04 measured/nominal
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Method : Method/Guideline - U.S. EPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975.

Statistical methods - Moving average angle, Probit or Bionomial Concentration.

Result : 48 hr EC50 >0.062 mg/L (based upon time zero analytical samples; no effects at test substance saturation; results from second study). Value was recalculated as >0.04 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Two studies were conducted because the initial test resulted in daphnids becoming trapped on the surface in the four highest test treatment levels and exhibiting immobility from this physical effect and therefore, the study was invalidated. Entrapment of daphnids suggested that the treatment solutions contained unsolubilized test substance. A repeat study included a control and only one high concentration with the nominal loading at a level that exceeded the water solubility of the test substance. The exposure solutions were prepared in a manner to avoid or minimize the possibility of test material in excess of saturation.

First Test:
Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25 mg/L.
Mean measured test concentrations of time 0 and 48 hr values: <0.0096,

0.014, 0.023, 0.037, 0.082, and 0.122 mg/L

Second Test:
Nominal test concentrations: control and 10 ul/L (saturated solution). Mean measured test concentrations of time 0 and 48 hr values: <0.015 and 0.04 mg/L. Mean measured values were used in the final EC50 calculation.

No immobility was observed after 48 hours in the repeat test although some, but not all daphnids were reported as caught on the surface in the treatment solution.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.

% Immobility results at 48 hrs per replicate for control and treatment levels in the first test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 0
0.014	0 / 0 / 0
0.023	0 / 0 / 20
0.037	100 / 100 / 100
0.082	80 / 80 / 100
0.122	80 / 100 / 100

More than 50% of the organisms were trapped on the surface of the 4 higher treatment solutions. Consequently, the study was repeated as a limit test using a saturated treatment solution.

% Immobility results at 48 hrs per replicate for control and treatment levels in the second limit test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 0
0.04	0 / 0 / 0

Data from the second test are used to characterize the acute toxicity of the test substance.

Test condition : Test treatments for the initial test were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the first test:
Test temperature = 21 Deg C. The pH ranged from 7.8 to 8.4 at initiation and 8.1 to 8.5 on day 2. Dissolved oxygen ranged from 8.8 to 9.0 at initiation and 7.7 to 7.9 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test treatments for the repeat study were prepared by mixing the test substance and 3 L of dilution water (fortified well water) on a magnetic stirrer for 1 hour at a loading of 9.7 mg/L, with a 50% vortex. After mixing the treatment solution was allowed to stand for 1 hour after which 2.5 L of solution was drained from the bottom of the flask into a glass bottle. The solution was allowed to stand for 24 hours after which 2.0 L was drained from the bottom into the test flasks and samples removed for analysis.

Three replicates of five organisms were tested. Test vessels were 250 ml beakers with 200 ml of test solution. Control test vessels were prepared under the same conditions but without test substance. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the second test:
Test temperature = 21 Deg C. The pH ranged from 8.0 to 8.1 at initiation and 8.3 to 8.4 on day 2. Dissolved oxygen was 7.9 at initiation and ranged from 7.0 to 7.6 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test substance : 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear (CAS# 111381-90-9)
Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.

Conclusion : Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

27.04.2006 (9) (12)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint :
Exposure period : 7 day(s)
Unit : mg/l
NOEC : = 1.6
EC50 : > 1.6 measured/nominal
Limit test :
Analytical monitoring : yes
Method : other
Year : 1978
GLP : yes
Test substance : other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Method : Method/Guideline - EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978.
Statistical methods - Moving average angle, Probit or Bionomial
Test type - Static

Result : 168 hr (7 day) EC50 >2.6 mg/L (based upon time zero analytical samples). Value was recalculated as >1.6 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentration as a percent of a saturated solution: 0 (control) and 100.0%.
Mean measured test concentrations of time 0 and 168 hr values: <0.10 and 1.6 mg/L (detection limit was 0.10 mg/L).

Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change. Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. A stimulatory effect

of 3 and 4% as compared with the control for chlorophyll a was measured on days 1 and 6, respectively. Analytical samples were taken at time zero and on a composite of replicates at termination.

Chlorophyll a percent change relative to control on sampling days and cell number on day 7 results:
Conc. Chlorophyll a percent change from control
(mg/L) Day 1 Day 2 Day 4 Day 6 Day 7 Cell # Day 7

1.6 +3 -6 -8 +4 -10 -4

Test condition : Algal Growth Medium was used as the control and diluent. 10 uL of test substance was added to 1.0 L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0 E4 cells/ml. Only one treatment level was evaluated (100%WSF) because earlier phthalate testing suggested that toxic effects were not expected with higher molecular weight phthalate esters with low water solubility.

Lighting = 4,700 lux, Test temperature = 22+/-2 Deg C. The pH was 7.5 at initiation and ranged from 7.9 to 8.2 on day 7. Algal culture stock was obtained from University of Texas at Austin, TX.

Test substance : 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear (CAS# 111381-90-9)
Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.

Conclusion : Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al (1997).

Reliability : (1) valid without restriction
The study procedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances. Control and exposure chlorophyll a or cell counts not reported.

Flag : Critical study for SIDS endpoint
27.04.2006 (10) (12)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species : Oncorhynchus mykiss (Fish, fresh water)
Endpoint : other: Early Life Stage Toxicity Test
Exposure period : 120 day(s)
Unit : mg/l
NOEC : = .41
Analytical monitoring : yes
Method : other
Year :
GLP : yes
Test substance : other TS: Di-(heptyl, nonyl, undecyl) Phthalate Ester (CAS No. 111381-90-9)

Method : Testing procedures followed the US Environmental Protection Agency, Toxic Substance Control Act (EPA-TSCA) 40 CFR, Part 797.1600 as modified in Testing Consent Agreement 40 CFR, Part 799 (1989), and the American Society for Testing and Materials (ASTM) Standard Guide for

Conducting Early Life-Stage Toxicity Tests with Fishes (1990).

Remark : Year: 1989; 1990

Result : Egg hatchability/survival, fry survival, and growth (length and weight) were evaluated as the biological endpoints. Di-(hepty, nonyl, undecyl) phthalate ester showed no effect on hatchability, survival, or growth at its highest achievable water solubility (0.41 mg/L) under the conditions of this test.

No sublethal physical and/or behavioral effects were noted at any test concentrations and no indications of feeding behavior changes in response to aeration of the test aquaria were noted.

Hatching started on day 28 and was 100% complete on day 32. Hatching success was 100% in control, solvent blank and exposure solutions.

Test material concentrations were confirmed on day -2, -1, 0, 1, 7, and weekly thereafter. Nominal loading levels were 0.038, 0.075, 0.15, 0.30, and 0.60 mg/L, which produced mean measured concentrations of 0.024, 0.044, 0.081, 0.18, and 0.41 mg/L, respectively.

The percent hatch of embryos in the control, solvent blank, and exposure levels was 100%

The percent survival of fish 60 days post-hatch exposure were 100 and 98% in the control and solvent blank, respectively, and 95 to 100% in the five exposure levels.

The percent survival of fish 91 days post-hatch exposure were 100 and 98% in the control and solvent blank, respectively, and 95 to 100% in the five exposure levels.

The percent survival of fish 120 days post-hatch exposure were 100 and 98% in the control and solvent blank, respectively, and 95 to 100% in the five exposure levels.

The mean standar length of fish after 60 days post-hatch was 51.4 and 50.24 mm in the control and solvent control, respectively, and 51.1 to 54.7 mm in the five exposure levels.

The mean standar length of fish after 91 days post-hatch was 76.4 and 75.4 mm in the control and solvent control, respectively, and 76.1 to 81.3 mm in the five exposure levels.

The mean standar length of fish after 120 days post-hatch was 103.2 and 102.5 mm in the control and solvent control, respectively, and 101.0 to 108.4 mm in the five exposure levels.

The mean blotted wet weight of fish after 120 days post-hatch was 18.3 and 17.8 g in the control and solvent control, respectively, and 16.9 to 20.9 g in the five exposure levels.

Test condition : The study used a flow-through test system. Test substance exposure solutions were prepared by mixing an appropriate amount of test substance into acetone (carrier solvent) to form a diluter stock solution. Control systems received an amount of carrier solvent approximately equivalent to the highest exposure concentration. The diluter stock solution was metered into a diluter chemcial mixing cell with a syringe injector. A sonicator was incorporated into mixing cell that received stock solution from the proportional diluter. Exposure solution then flowed to the test systems.

In the high exposures, small droplets of test substance formed, which were physically removed by skimming the medium surface during the diluter cycle.

At study initiation, 40 to 60 Oncorhynchus mykiss embryos were impartially distributed into smaller incubation chambers that were suspended in each test system. The incubation chambers were mechanically oscillated vertically in each test system by a rocker arm to facilitate test solution circulation and to keep the embryos clean.

On day 25, embryos were impartially redued to 20 eyed embryos in each chamber. After hatch (35 days post fertilization) sac-fry were released from the incubation chambers into the test system. Developing embryos were maintained under low light through hatch. After hatch, a 14:10 hour light:dark photoperid with a simulated dawn and dush transition period was maintained. Light intensity over the test systems during the day photoperiod was approximately 50 lumens/ft2.

Beginning at the start of swim-up, fish were fed a comercially prepared Salmon Starter® (Zeigler Bros, Gardners, PA, USA) in combination with live brine shrimp mauplii (Artemia sp.). Fish were fed two to three times a day. Test systems were siphoned daily during the growth phase to remove fecal material and uneaten food and to minimize microbial growth.

Towards test termination, pure oxygen was added to the dilution water as it entered the diluter system to maintain acceptable oxygen concentrations in the test systems. In addition, on day 144, gentle aeration directly in the test systems was initiated to further ensure adequate oxygen levels were maintained. The additional oxygenation procedures were necessitated due to the growth of the fish.

The total exposure time was 155 days, 120 days post-hatch.

At test termination, standard length of fish was determined photographically, after which fish were sacrificed and measured again for length and dry-blotted wet weight.

Water quality measurements were determined periodically during the tests in one or more replicates at intervals ranging from once daily to once weekly. Test conditions during incubation and growth were:

Temperature = 10 +/- 1.5 degree C during egg incubation
Temperature = 12 +/- 1.5 degree C during growth phase
Water harness = 158 to 198 mg/L (as CaCO3)
Alkalinity = 117 to 216 mg/L (as CaCO3)
pH = 7.0 to 8.6

Test substance analyses of exposure solutions were performed using gas chromatography. The mean measured water exposure concentrations were: control (below minimum detectable level), 0.024 (SD 0.0087), 0.044 (SD 0.010), 0.081 (SD 0.021), 0.180 (SD 0.035), 0.410 (SD 0.120).

Test substance : The test was conducted using a uniformly ring-labeled 14C-di-(heptyl, nonyl, undecyl) phthalate ester that was >95% pure.

Conclusion : The chronic fish (Oncorhynchus mykiss) toxicity (early life-stage) data reported for di-(heptyl, nonyl, undecyl) phthalate are consistent with the data for several high molecular weight phthalate esters as summarized by Rhodes et al. (1995). These data clearly showed that high molecular weight phthalate esters, including di-(heptyl, nonyl, undecyl) phthalate, did not produce chronic toxicity to a fish at or below their maximum attainable water solubility.

Reliability : (1) valid without restriction
The study proceedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
27.04.2006

(1) (8)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Mouse lymphoma assay
System of testing	:	Mammalian Cell
Test concentration	:	0.125 to 6 ul/ml
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 476
Year	:	
GLP	:	yes
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear
Method	:	Control Group: The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9. Statistical Methods: The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10 x 10-6. The background frequency was defined as the average mutant frequency of the solvent negative controls.
Result	:	In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a

metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.

Test condition : Mouse lymphoma cells were seeded into a series of tubes at 6 x 106 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3 x 106 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.

Test substance : Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11).

Data used as read-across to 1,2-benzenedicarboxylic acid, heptyl undecyl ester. CAS #111381-90-9.

Conclusion : Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

05.07.2006 (2)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Wistar
Route of admin.	:	gavage
Exposure period	:	Gestation days 6-15
Frequency of treatm.	:	Daily
Duration of test	:	9 days
Doses	:	0, 40, 200, 1000 mg/kg/day.
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 200 mg/kg bw
NOAEL teratogen.	:	= - 200 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	
GLP	:	yes
Test substance	:	other TS: CAS #111381-90-9; 1,2-benzenedicarboxylic acid, heptyl undecyl ester, branched and linear

Method : Statistical Methods: Dunnett's Test for food consumption, body weight, organ weight, placental and fetal data; Fisher's Exact Test for female mortality, litters with findings; and the Wilcoxon Test for proportion of fetuses with findings per litter.

Result	:	Maternal Effects: There were no treatment-related effects in the 40 or 200 mg/kg/day groups either in the dams or fetuses. The high dose (1000 mg/kg/day) maternal body weights were decreased during gestation days 15-20, and relative liver and kidney weight was increased in the high dose group dams. Six of the ten high dose dams showed vaginal hemorrhage during the study; three had complete resorptions. Embryo/Fetal Effects: Fetal weights of the remaining viable litters were reduced, and all litters contained malformations. The malformations affected mainly the brain, vertebral column, tail, scapula, sternum, and urogenital tract. In total, 47/53 high-dose fetuses (89%) from all seven litters were malformed.
Test condition	:	Eight to ten pregnant females were used per group. Animals were weighed on gestation days 0, 6, 10, 15, and 20, and observed daily for signs of toxicity. On GD 20, animals were sacrificed and maternal body, liver, kidneys, and intact uterus were weighed. Fetuses were weighed, examined for external and visceral abnormalities.
Test substance	:	Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11). Data used as read-across to 1,2-benzenedicarboxylic acid, heptyl undecyl ester. CAS #111381-90-9.
Conclusion	:	Significant maternal and fetal effects only were observed at the high dose (1000 mg/kg/day). No treatment-related effects were observed in the 40 or 200 mg/kg/day groups.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint
05.07.2006		(6)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) ABC, Analytical Bio Chemistry Labs, Inc. (1991). Early Life-stage Toxicity of Di(heptyl, nonyl, undecyl) Phthalate (D711P) to the Rainbow Trout (Oncorhynchus mykiss) Under Flow-through Conditions. Study performed for CMA (Chemical Manufactures Association), Washington, DC, USA.

(2) Barber E, Cifone M, Rundell J, Przygoda R, Astill B, Moran E, Mulholland A, Robinson E and Schneider B (1999). Results in the L5178Y mouse lymphoma and the in vitro transformation of Balb 3T3 cell assays for eight phthalate esters. Journal of Applied Toxicology 20, 69-80.

(3) Cousins I and Mackay D (2000). Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. Chemosphere 41, 1389-1399.

(4) EG&G Bionomics, Inc. (1983). Acute Toxicity of Fourteen Esters to Rainbow Trout Salmo gairdneri Under Flow-Through Conditions. Report No. BW-83-3-1373. Unpublished report.

(5) Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.

(6) Hellwig J, Freudenberger H and Jackh R (1997). Differential prenatal toxicity of branched phthalate esters in rats. Food and Chemical Toxicology 35, 501-512.

(7) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

(8) Rhodes J, Adams W, Biddinger G, Robillard K and Gorsuch J (1995). Chronic toxicity of 14 phthalate esters to Daphnia magna and Rainbow trout (Oncorhynchus mykiss). Environ Toxicol Chem 14, 1967-1976.

(9) Springborn Bionomics, Inc. (1984). Acute Toxicity of Fourteen Esters to Daphnia magna. Report No. BW-84-4-1567. Unpublished report.

(10) Springborn Bionomics, Inc. (1984). Acute Toxicity of Fourteen Esters to the Freshwater Green Alga Selenastrum capricornutum. Report No. BP-84-1-4. Unpublished report.

(11) Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. Chemosphere 35, 667-749.

(12) Staples CA, et al (1997). Aquatic toxicity of eighteen phthalate esters. Environmental Toxicology and Chemistry 16(5), 875-891.

(13) Sugatt RH, et al (1983). Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY, USA. SRC# L1543-05. Performed for CMA.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

05.07.2006

10.3 RISK ASSESSMENT